In the Claims: Please amend claims 2 and 13 as follows:

1. (Cancelled)

2. (Currently amended) A computer-assisted method for predicting the binding affinity of a compound for a binding target of a molecule, using a programmed computer including a processor, an input device, and an output device, including the steps of:

~~(a) inputting into the programmed computer, through the input device, data including the identity and three-dimensional coordinates of each of the atoms in the binding target, wherein the binding target has been selected from a plurality of predicted binding targets generated by~~

i) inputting into the programmed computer, through the input device, data including the identity and three-dimensional coordinates of each of the atoms in the molecule;

ii) determining, using the processor, for each atom in the molecule, a predicted Gibbs free energy of binding of the atom to an ideal ligand ~~for the atom~~;

iii) generating, using the processor, a three-dimensional prediction model of binding targets in the molecule by generating, using the three-dimensional coordinates of each of the atoms in the molecule, a model of the atoms in the molecule and mapping onto each atom depicted in the model the corresponding determined predicted Gibbs free energy of binding; ~~said generating step yielding data including the identity and three-dimensional coordinates of each of the atoms in the binding target which will be input into the programmed computer;~~

iv) identifying as a binding target a region of the molecule with a high density of atoms which exhibit favorable Gibbs free energy of binding to said ideal ligand,

v) inputting into the programmed computer, through the input device, data including the identity and three-dimensional coordinates of each of the atoms in the binding target,

~~(b)~~ vi) inputting into the programmed computer, through the input device, data including the identity and three-dimensional coordinates of each of the atoms in the compound;

~~(c)~~ vii) generating, using the processor, a model of the compound bound to the binding target;

~~(d)~~ viii) determining, using the processor, the three-dimensional coordinates of an energy minimized structure of the compound when the compound is bound to the binding target; and

~~(c)~~ ix) determining, using the processor, a predicted binding affinity of the energy minimized compound for the binding target.

3-12. (Cancelled)

13. (Currently amended) A computer program, residing on a computer-readable medium, for predicting the binding affinity of a compound for a binding target of a molecule, the computer program including instructions for causing a computer to:

~~(a) receive data including the identity and three-dimensional coordinates of each of the atoms in the binding target; wherein the binding target has been selected from a plurality of predicted binding targets generated by~~

i) ~~inputting into a programmed computer, through an input device,~~ receive data including the identity and three-dimensional coordinates of each of the atoms in the molecule;

ii) ~~determining, using a processor~~ determine, for each atom in the molecule, a predicted Gibbs free energy of binding of the atom to an ideal ligand for the atom;

iii) ~~generating, using the processor~~ generate a three-dimensional prediction model of binding targets in the molecule by generating, using the three-dimensional coordinates of each of the atoms in the molecule, a model of the atoms in the molecule and mapping onto each atom depicted in the model the corresponding determined predicted Gibbs free energy of binding; ~~said generating step yielding data including the identity and three-dimensional coordinates of each of the atoms in the binding target which will be input into the programmed computer;~~

iv) identify as a binding target a region of the molecule with a high density of atoms which exhibit favorable Gibbs free energy of binding to said ideal ligand,

~~(a)~~ v) receive data including the identity and three-dimensional coordinates of each of the atoms in the binding target; ~~wherein the binding target has been selected from a plurality of predicted binding targets generated by~~

~~(b)~~ vi) receive data including the identity and three-dimensional coordinates of each of the atoms in the compound;

~~(c)~~ vii) generate a model of the compound bound to the binding target;

~~(d)~~ viii) determine the three-dimensional coordinates of an energy minimized structure of the compound when the compound is bound to the binding target; and

~~(e)~~ ix) determine a predicted binding affinity of the energy minimized compound for the binding target.

14 -17. (Cancelled)